



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:25 AM UTC

PDB ID : 3IQZ / pdb_00003iqz
Title : Structure of F420 dependent methylene-tetrahydromethanopterin dehydrogenase in complex with methylene-tetrahydromethanopterin
Authors : Ceh, K.E.; Demmer, U.; Warkentin, E.; Moll, J.; Thauer, R.K.; Shima, S.; Ermler, U.
Deposited on : 2009-08-21
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

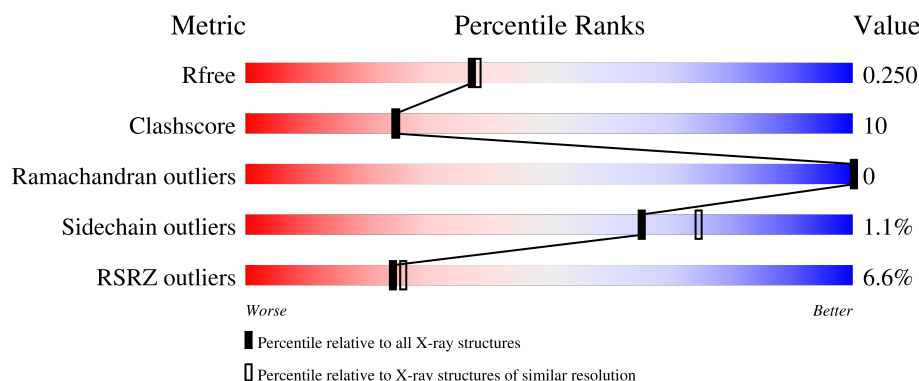
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	17% 88% 12%
1	B	283	3% 83% 16%
1	C	283	4% 82% 18%
1	D	283	13% 85% 14%

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Mol	Chain	Length	Quality of chain
1	E	283	% 80% 19%
1	F	283	% 83% 16%

2 Entry composition ⓘ

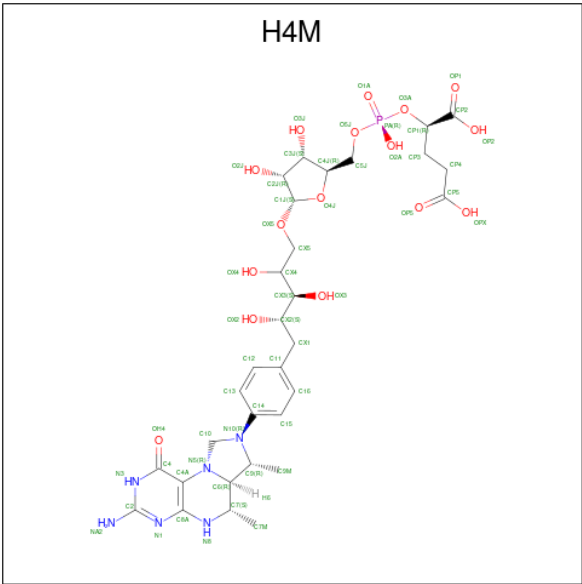
There are 6 unique types of molecules in this entry. The entry contains 13675 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called F420-dependent methylenetetrahydromethanopterin dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2187	1373	357	437	20			
1	B	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	C	282	Total	C	N	O	S	0	3	0
			2202	1382	358	442	20			
1	D	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	E	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	F	282	Total	C	N	O	S	0	1	0
			2188	1373	357	439	19			

- Molecule 2 is 5,10-DIMETHYLENE TETRAHYDROMETHANOPTERIN (CCD ID: H4M) (formula: C₃₁H₄₅N₆O₁₆P).

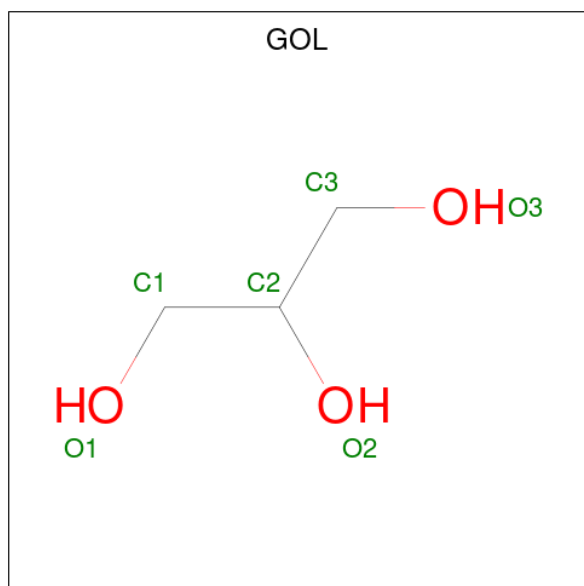


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	B	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	C	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	D	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	E	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	F	1	Total	C	N	O	P	0	0
			45	26	6	12	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Na 1	0	0
5	E	1	Total 1	Na 1	0	0
5	F	1	Total 1	Na 1	0	0

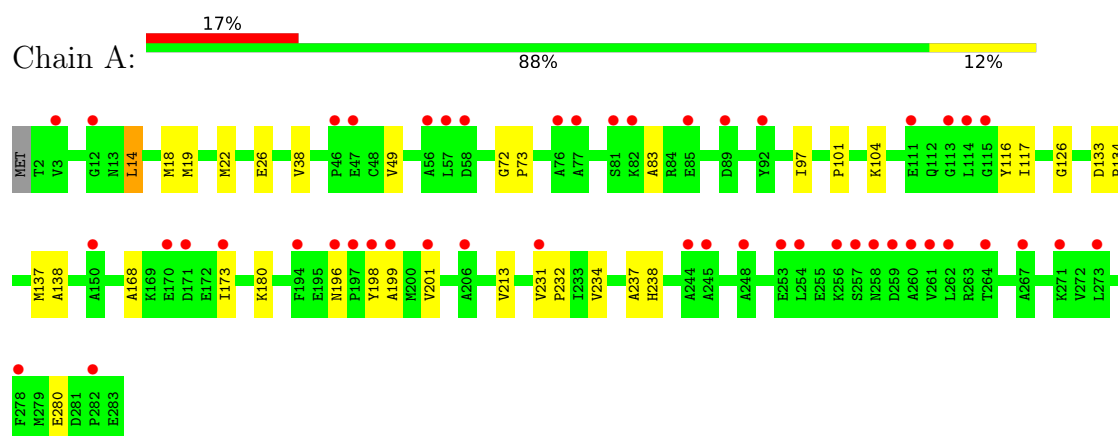
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total 29	O 29	0	0
6	B	79	Total 79	O 79	0	0
6	C	56	Total 56	O 56	0	0
6	D	18	Total 18	O 18	0	0
6	E	42	Total 42	O 42	0	0
6	F	48	Total 48	O 48	0	0

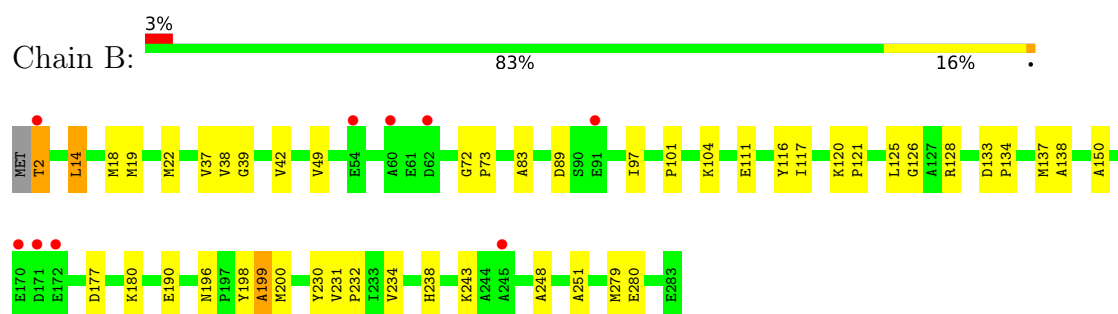
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

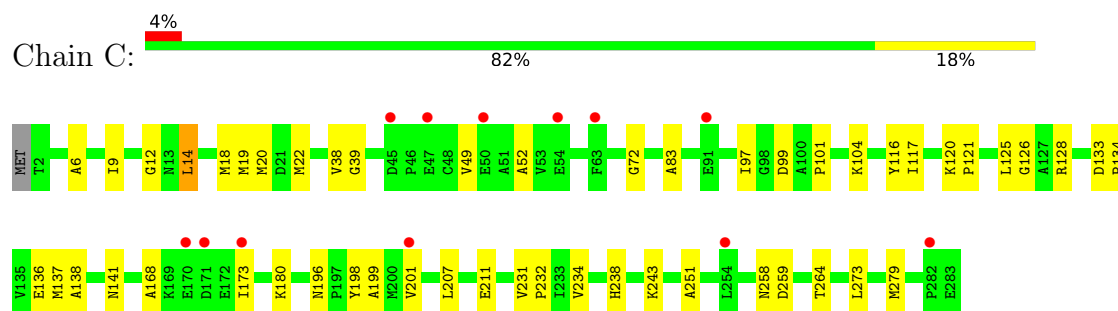
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



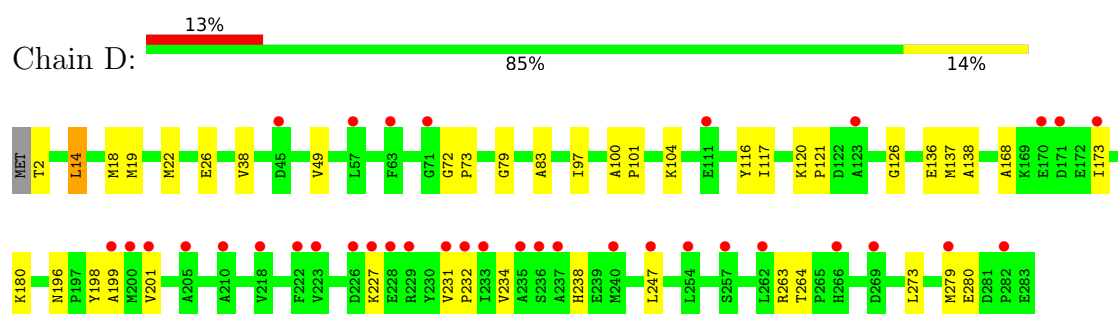
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



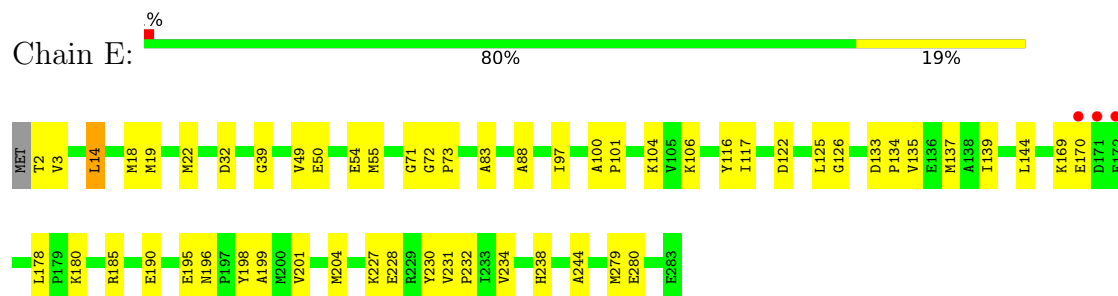
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



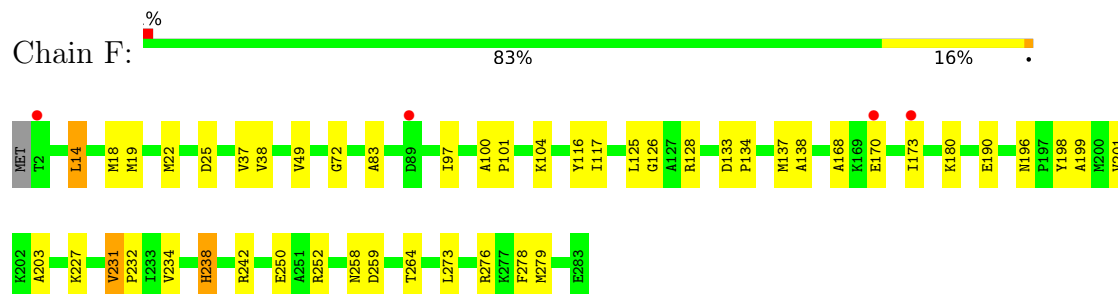
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.81Å 167.70Å 95.86Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	94.00 – 2.10 94.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (94.00-2.10) 96.9 (94.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.198 , 0.226 0.222 , 0.250	Depositor DCC
R_{free} test set	5502 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13675	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, H4M, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/2223	0.89	0/2999
1	B	1.12	4/2215 (0.2%)	1.04	1/2989 (0.0%)
1	C	1.03	3/2241 (0.1%)	0.99	2/3023 (0.1%)
1	D	0.78	0/2215	0.89	0/2989
1	E	0.98	1/2215 (0.0%)	1.07	2/2989 (0.1%)
1	F	1.04	3/2224 (0.1%)	1.01	2/3001 (0.1%)
All	All	0.96	11/13333 (0.1%)	0.98	7/17990 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	203	ALA	CA-CB	7.17	1.65	1.53
1	B	251	ALA	CA-CB	6.81	1.64	1.53
1	C	6	ALA	CA-CB	6.40	1.65	1.53
1	B	128	ARG	C-O	6.06	1.31	1.24
1	C	52	ALA	CA-CB	5.92	1.62	1.53
1	B	199	ALA	C-O	5.81	1.30	1.24
1	F	231	VAL	CA-CB	5.81	1.57	1.54
1	E	244	ALA	CA-CB	5.31	1.61	1.53
1	F	252	ARG	N-CA	-5.28	1.40	1.46
1	C	251	ALA	CA-CB	5.25	1.61	1.53
1	B	200	MET	N-CA	5.16	1.52	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	TYR	N-CA-C	6.35	119.01	111.71
1	F	242	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	C	20	MET	N-CA-C	5.66	117.90	111.11
1	E	178	LEU	CA-C-N	-5.38	114.24	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	178	LEU	C-N-CA	-5.38	114.24	119.78
1	C	12	GLY	N-CA-C	-5.25	103.14	112.58
1	F	238	HIS	N-CA-C	5.10	116.84	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2187	0	2166	45	0
1	B	2182	0	2157	50	2
1	C	2202	0	2177	57	0
1	D	2182	0	2157	46	0
1	E	2182	0	2157	56	3
1	F	2188	0	2163	50	2
2	A	45	0	37	8	0
2	B	45	0	37	0	0
2	C	45	0	37	12	0
2	D	45	0	37	6	0
2	E	45	0	37	1	0
2	F	45	0	37	7	0
3	B	1	0	0	0	1
4	B	6	0	8	3	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	29	0	0	0	0
6	B	79	0	0	8	0
6	C	56	0	0	1	0
6	D	18	0	0	1	0
6	E	42	0	0	5	0
6	F	48	0	0	2	0
All	All	13675	0	13207	261	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:MET:CE	1:F:22:MET:HE1	1.56	1.34
1:C:137[B]:MET:CE	1:E:19:MET:HE1	1.65	1.25
4:B:286:GOL:C3	6:B:365:HOH:O	1.86	1.24
1:C:137[B]:MET:HE1	1:E:19:MET:CE	1.70	1.22
1:A:18:MET:CE	1:D:22:MET:HE1	1.72	1.19
1:A:18:MET:HE3	1:D:22:MET:HE1	1.22	1.14
1:C:22:MET:HE1	1:E:18:MET:HE3	1.28	1.13
1:B:22:MET:HE1	1:F:18:MET:CE	1.79	1.12
1:A:22:MET:HE1	1:D:18:MET:CE	1.81	1.10
1:A:137[B]:MET:HE2	2:A:284:H4M:H4	1.06	1.10
1:C:22:MET:HE1	1:E:18:MET:CE	1.81	1.10
1:B:18:MET:HE3	1:F:22:MET:HE1	1.18	1.08
2:A:284:H4M:H9	1:D:26:GLU:O	1.54	1.07
4:B:286:GOL:H32	6:B:365:HOH:O	1.49	1.07
1:C:18:MET:HE3	1:E:22:MET:HE1	1.35	1.05
1:A:22:MET:HE1	1:D:18:MET:HE3	1.37	1.04
2:D:284:H4M:H18	2:D:284:H4M:H12	1.42	1.01
1:B:22:MET:HE1	1:F:18:MET:HE3	1.40	1.00
1:C:137[B]:MET:HE1	1:E:19:MET:HE1	1.00	0.97
1:C:18:MET:CE	1:E:22:MET:HE1	1.94	0.95
1:B:18:MET:HE1	1:F:22:MET:HE1	1.43	0.95
1:C:137[A]:MET:HE3	2:C:284:H4M:H4	1.31	0.95
1:B:18:MET:CE	1:F:22:MET:CE	2.44	0.95
1:C:137[A]:MET:CE	2:C:284:H4M:H4	1.79	0.95
1:A:19:MET:HE1	1:D:137:MET:HE1	1.49	0.93
1:E:126:GLY:H	1:E:238:HIS:HE1	1.12	0.92
1:D:126:GLY:H	1:D:238:HIS:HE1	1.18	0.92
1:B:19:MET:HE1	1:F:137:MET:HE1	1.52	0.92
1:B:137:MET:HE1	1:F:19:MET:HE1	1.51	0.91
4:B:286:GOL:H31	6:B:365:HOH:O	1.58	0.91
1:C:207:LEU:O	1:C:211[B]:GLU:HG3	1.71	0.90
1:B:22:MET:HE1	1:F:18:MET:HE1	1.54	0.89
1:B:126:GLY:H	1:B:238:HIS:HE1	1.18	0.89
1:A:126:GLY:H	1:A:238:HIS:HE1	1.21	0.88
1:C:126:GLY:H	1:C:238:HIS:HE1	1.17	0.88
1:F:126:GLY:H	1:F:238:HIS:HE1	1.19	0.88
1:E:279:MET:HA	1:E:279:MET:HE3	1.57	0.87
1:A:137[B]:MET:HE2	2:A:284:H4M:N8	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:MET:CE	1:E:18:MET:CE	2.58	0.81
1:C:19:MET:HE1	1:E:137:MET:HE1	1.62	0.81
1:A:18:MET:CE	1:D:22:MET:CE	2.58	0.80
1:C:137[A]:MET:HE2	1:C:141:ASN:ND2	1.98	0.79
1:A:101:PRO:O	1:A:104:LYS:HE3	1.82	0.79
1:C:22:MET:CE	1:E:18:MET:HE3	2.12	0.78
1:B:111:GLU:HG3	6:B:325:HOH:O	1.83	0.78
1:F:276:ARG:O	6:F:288:HOH:O	2.00	0.78
1:A:22:MET:HE1	1:D:18:MET:HE1	1.63	0.77
2:F:284:H4M:C10	2:F:284:H4M:OH4	2.33	0.76
1:F:196:ASN:HD22	1:F:199:ALA:H	1.31	0.75
1:E:126:GLY:H	1:E:238:HIS:CE1	2.02	0.74
1:A:18:MET:HE1	1:D:22:MET:HE1	1.66	0.74
2:F:284:H4M:O2A	6:F:297:HOH:O	2.04	0.74
1:C:137[A]:MET:HE2	1:C:141:ASN:HD21	1.50	0.74
1:D:196:ASN:HD22	1:D:199:ALA:H	1.35	0.73
1:B:18:MET:HE3	1:F:22:MET:CE	2.09	0.73
2:A:284:H4M:C7M	1:D:26:GLU:O	2.34	0.73
1:E:116:TYR:CE1	1:E:180:LYS:HG2	2.23	0.73
1:B:22:MET:CE	1:F:18:MET:CE	2.65	0.73
1:C:18:MET:HE3	1:E:22:MET:CE	2.17	0.73
1:C:22:MET:HE1	1:E:18:MET:HE1	1.69	0.73
1:E:88:ALA:O	6:E:320:HOH:O	2.06	0.72
1:E:126:GLY:N	1:E:238:HIS:HE1	1.87	0.72
1:B:137:MET:CE	1:F:19:MET:HE1	2.19	0.72
1:C:196:ASN:HD22	1:C:199:ALA:H	1.38	0.71
2:D:284:H4M:H12	2:D:284:H4M:C13	2.18	0.70
1:E:101:PRO:O	1:E:104:LYS:HE3	1.92	0.70
1:A:196:ASN:HD22	1:A:199:ALA:H	1.39	0.70
1:C:18:MET:CE	1:E:22:MET:CE	2.70	0.70
1:B:18:MET:HE1	1:F:22:MET:CE	2.15	0.69
1:A:22:MET:CE	1:D:18:MET:CE	2.65	0.69
1:E:196:ASN:HD22	1:E:199:ALA:H	1.40	0.69
1:B:196:ASN:HD22	1:B:199:ALA:H	1.38	0.68
1:F:101:PRO:O	1:F:104:LYS:HE3	1.94	0.68
1:B:19:MET:HE1	1:F:137:MET:CE	2.24	0.67
1:B:101:PRO:O	1:B:104:LYS:HE3	1.95	0.67
1:F:126:GLY:H	1:F:238:HIS:CE1	2.09	0.66
1:B:14:LEU:HD22	1:B:72:GLY:C	2.21	0.65
1:F:279:MET:HE3	1:F:279:MET:HA	1.79	0.64
1:C:279:MET:HE3	1:C:279:MET:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137[A]:MET:HE1	1:D:19:MET:HE1	1.79	0.63
1:D:101:PRO:O	1:D:104:LYS:HE3	1.97	0.63
1:E:195:GLU:OE2	6:E:323:HOH:O	2.14	0.63
2:F:284:H4M:H18	2:F:284:H4M:H12	1.80	0.63
1:C:137[A]:MET:HE2	2:C:284:H4M:H4	1.64	0.63
1:C:101:PRO:O	1:C:104:LYS:HE3	1.99	0.63
1:C:126:GLY:HA3	1:C:234:VAL:HB	1.80	0.62
2:C:284:H4M:C13	2:C:284:H4M:H12	2.29	0.62
1:B:22:MET:CE	1:F:18:MET:HE1	2.25	0.62
2:D:284:H4M:C10	2:D:284:H4M:OH4	2.48	0.62
1:A:18:MET:HE3	1:D:22:MET:CE	2.14	0.61
2:F:284:H4M:OH4	2:F:284:H4M:H15	2.00	0.61
1:B:126:GLY:H	1:B:238:HIS:CE1	2.09	0.61
1:E:2:THR:HG22	1:E:3:VAL:N	2.16	0.61
1:A:19:MET:HE1	1:D:137:MET:CE	2.29	0.61
2:C:284:H4M:H12	2:C:284:H4M:H18	1.84	0.60
1:A:22:MET:CE	1:D:18:MET:HE3	2.25	0.59
1:A:137[A]:MET:SD	1:D:19:MET:HE1	2.43	0.59
1:C:19:MET:HE1	1:E:137:MET:CE	2.33	0.59
2:C:284:H4M:C10	2:C:284:H4M:OH4	2.49	0.59
1:D:231:VAL:HB	1:D:232:PRO:HD3	1.85	0.59
1:D:126:GLY:H	1:D:238:HIS:CE1	2.10	0.58
1:B:73:PRO:HG2	6:B:317:HOH:O	2.03	0.58
1:E:198:TYR:HA	1:E:201:VAL:HG22	1.84	0.58
1:A:231:VAL:HB	1:A:232:PRO:HD3	1.86	0.58
1:B:38:VAL:HG12	1:F:38:VAL:HG12	1.86	0.58
1:C:137[B]:MET:CE	1:E:19:MET:CE	2.49	0.57
1:E:101:PRO:HG2	6:E:296:HOH:O	2.04	0.57
1:C:22:MET:CE	1:E:18:MET:HE1	2.30	0.56
1:A:126:GLY:HA3	1:A:234:VAL:HB	1.86	0.56
1:F:14:LEU:HD22	1:F:72:GLY:C	2.31	0.56
2:A:284:H4M:H12	2:A:284:H4M:H18	1.88	0.56
1:A:116:TYR:CE1	1:A:180:LYS:HG2	2.40	0.56
1:B:279:MET:HE3	1:B:279:MET:HA	1.88	0.56
1:C:133:ASP:HB2	1:C:134:PRO:CD	2.37	0.55
1:F:126:GLY:HA3	1:F:234:VAL:HB	1.88	0.55
1:F:116:TYR:CE1	1:F:180:LYS:HG2	2.42	0.55
1:F:128:ARG:HH21	2:F:284:H4M:H33	1.71	0.55
1:C:126:GLY:H	1:C:238:HIS:CE1	2.09	0.55
1:E:133:ASP:HB2	1:E:134:PRO:CD	2.36	0.54
1:A:26:GLU:O	2:D:284:H4M:H9	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:THR:N	6:B:349:HOH:O	2.41	0.54
1:D:263:ARG:NE	6:D:289:HOH:O	2.34	0.54
1:F:128:ARG:NH2	2:F:284:H4M:H33	2.21	0.54
1:A:126:GLY:H	1:A:238:HIS:CE1	2.13	0.54
1:C:137[A]:MET:HE3	2:C:284:H4M:N8	2.11	0.54
1:B:111:GLU:CG	6:B:325:HOH:O	2.51	0.53
1:E:14:LEU:HD13	1:E:73:PRO:HG3	1.90	0.53
1:A:137[A]:MET:CE	1:D:19:MET:HE1	2.39	0.53
1:E:116:TYR:CZ	1:E:180:LYS:HG2	2.44	0.53
1:B:116:TYR:CE1	1:B:180:LYS:HG2	2.43	0.53
2:D:284:H4M:H18	2:D:284:H4M:C9M	2.19	0.53
1:B:126:GLY:N	1:B:238:HIS:HE1	1.98	0.52
1:C:116:TYR:CE1	1:C:180:LYS:HG2	2.44	0.52
1:B:14:LEU:HD13	1:B:73:PRO:HG3	1.91	0.52
1:E:106:LYS:HE2	6:E:293:HOH:O	2.08	0.52
1:A:196:ASN:ND2	1:A:198:TYR:H	2.08	0.52
1:C:18:MET:HE1	1:E:22:MET:HE1	1.83	0.52
1:F:97:ILE:HD12	1:F:117:ILE:HB	1.91	0.51
1:A:22:MET:CE	1:D:18:MET:HE1	2.33	0.51
1:A:196:ASN:HD21	1:A:198:TYR:HB2	1.75	0.51
1:C:258:ASN:O	1:C:259:ASP:C	2.54	0.51
1:C:136:GLU:OE1	1:C:238:HIS:HD2	1.94	0.51
1:E:100:ALA:N	1:E:101:PRO:CD	2.74	0.51
1:E:126:GLY:HA3	1:E:234:VAL:HB	1.93	0.51
1:F:196:ASN:HD21	1:F:198:TYR:HB2	1.75	0.50
1:C:14:LEU:HD22	1:C:72:GLY:C	2.36	0.50
1:C:128:ARG:NH2	2:C:284:H4M:H33	2.26	0.50
1:C:137[A]:MET:CE	1:C:141:ASN:ND2	2.72	0.50
1:D:116:TYR:CE1	1:D:180:LYS:HG2	2.47	0.50
1:A:14:LEU:HD22	1:A:72:GLY:C	2.37	0.50
1:D:126:GLY:HA3	1:D:234:VAL:HB	1.93	0.50
1:E:279:MET:HA	1:E:279:MET:CE	2.36	0.50
2:F:284:H4M:H12	2:F:284:H4M:C13	2.40	0.50
1:A:19:MET:HE2	1:D:138:ALA:HB2	1.94	0.49
1:E:133:ASP:HB2	1:E:134:PRO:HD2	1.95	0.49
1:C:198:TYR:HA	1:C:201:VAL:HG22	1.95	0.49
1:C:97:ILE:HD12	1:C:117:ILE:HB	1.95	0.48
1:D:198:TYR:HA	1:D:201:VAL:HG22	1.95	0.48
1:A:138:ALA:HB2	1:D:19:MET:HE2	1.95	0.48
1:D:168:ALA:HB2	1:D:173:ILE:HD11	1.95	0.48
1:B:49:VAL:CG1	1:B:83:ALA:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ASP:OD1	1:E:169:LYS:NZ	2.44	0.48
1:C:264:THR:HA	1:C:273:LEU:O	2.14	0.48
1:A:137[A]:MET:HG3	2:A:284:H4M:H8	1.95	0.48
2:D:284:H4M:C13	2:D:284:H4M:C9M	2.83	0.47
1:E:279:MET:HE3	1:E:279:MET:CA	2.36	0.47
1:E:14:LEU:HD22	1:E:72:GLY:C	2.39	0.47
1:B:120:LYS:N	1:B:121:PRO:CD	2.78	0.47
1:C:49:VAL:CG1	1:C:83:ALA:HB2	2.44	0.47
1:C:168:ALA:HB2	1:C:173:ILE:HD11	1.96	0.47
1:C:231:VAL:HB	1:C:232:PRO:HD3	1.95	0.47
1:D:196:ASN:HD21	1:D:198:TYR:HB2	1.79	0.47
1:E:125:LEU:C	1:E:125:LEU:HD12	2.40	0.47
1:E:134:PRO:HD2	6:E:322:HOH:O	2.15	0.47
1:F:231:VAL:HB	1:F:232:PRO:HD3	1.96	0.47
1:A:198:TYR:HA	1:A:201:VAL:HG22	1.97	0.47
1:B:97:ILE:HD12	1:B:117:ILE:HB	1.96	0.47
1:C:18:MET:HE1	1:E:22:MET:CE	2.43	0.47
1:D:264:THR:HA	1:D:273:LEU:O	2.14	0.47
1:A:49:VAL:CG1	1:A:83:ALA:HB2	2.44	0.47
1:B:126:GLY:HA3	1:B:234:VAL:HB	1.97	0.47
1:A:116:TYR:CZ	1:A:180:LYS:HG2	2.50	0.47
1:E:135:VAL:O	1:E:139:ILE:HG13	2.15	0.47
1:A:38:VAL:HG12	1:D:38:VAL:HG12	1.97	0.46
1:B:39:GLY:HA3	6:B:326:HOH:O	2.14	0.46
1:D:14:LEU:HD22	1:D:72:GLY:C	2.40	0.46
1:C:137[B]:MET:HE3	1:C:138:ALA:N	2.30	0.46
1:C:137[A]:MET:CE	2:C:284:H4M:N8	2.62	0.46
1:B:231:VAL:HB	1:B:232:PRO:HD3	1.98	0.46
1:A:18:MET:HE1	1:D:22:MET:CE	2.37	0.46
1:D:279:MET:HE3	1:D:279:MET:HA	1.98	0.46
1:D:97:ILE:HD12	1:D:117:ILE:HB	1.96	0.46
1:E:50:GLU:O	1:E:54:GLU:HG3	2.17	0.45
1:B:125:LEU:C	1:B:125:LEU:HD12	2.42	0.45
1:B:42:VAL:HG21	1:F:25:ASP:O	2.17	0.45
1:E:185:ARG:HG3	1:E:204:MET:O	2.17	0.45
1:E:2:THR:HG22	1:E:3:VAL:H	1.80	0.45
1:A:168:ALA:HB2	1:A:173:ILE:HD11	1.98	0.45
1:F:168:ALA:HB2	1:F:173:ILE:HD11	1.99	0.45
1:B:116:TYR:CZ	1:B:180:LYS:HG2	2.51	0.45
1:A:137[B]:MET:HG3	2:A:284:H4M:H8	1.99	0.44
1:E:71:GLY:HA2	1:E:97:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:VAL:CG1	1:F:83:ALA:HB2	2.47	0.44
1:B:37:VAL:O	1:F:38:VAL:HA	2.16	0.44
1:D:100:ALA:N	1:D:101:PRO:CD	2.80	0.44
1:E:122:ASP:OD1	1:E:144:LEU:HD21	2.17	0.44
1:C:9:ILE:HA	1:C:38:VAL:O	2.18	0.44
1:C:19:MET:HE3	1:C:19:MET:HB3	1.43	0.44
1:D:49:VAL:HG11	1:D:79:GLY:O	2.18	0.44
1:E:19:MET:HE3	1:E:19:MET:HB3	1.87	0.44
1:E:49:VAL:CG1	1:E:83:ALA:HB2	2.48	0.44
1:F:100:ALA:N	1:F:101:PRO:CD	2.81	0.44
1:F:258:ASN:O	1:F:259:ASP:C	2.59	0.44
1:A:133:ASP:HB2	1:A:134:PRO:CD	2.48	0.43
1:E:39:GLY:O	1:E:55:MET:HE1	2.18	0.43
1:D:97:ILE:CD1	1:D:117:ILE:HB	2.48	0.43
2:E:284:H4M:OH4	2:E:284:H4M:C10	2.66	0.43
1:F:133:ASP:HB2	1:F:134:PRO:CD	2.48	0.43
1:F:264:THR:HA	1:F:273:LEU:O	2.18	0.43
1:B:231:VAL:HG12	1:F:278:PHE:CZ	2.54	0.43
1:E:2:THR:CG2	1:E:3:VAL:N	2.81	0.43
1:E:227:LYS:HA	1:E:230:TYR:CD1	2.54	0.43
1:E:231:VAL:HB	1:E:232:PRO:HD3	2.00	0.43
1:B:150:ALA:HB3	1:B:248:ALA:HB1	2.00	0.43
1:B:133:ASP:HB2	1:B:134:PRO:CD	2.49	0.43
2:C:284:H4M:OH4	2:C:284:H4M:H15	2.19	0.43
1:D:14:LEU:HD13	1:D:73:PRO:HG3	2.00	0.42
1:F:100:ALA:HB3	1:F:101:PRO:HD3	2.00	0.42
1:B:196:ASN:HD21	1:B:198:TYR:HB2	1.84	0.42
1:F:116:TYR:CZ	1:F:180:LYS:HG2	2.55	0.42
1:F:125:LEU:HD12	1:F:125:LEU:C	2.45	0.42
1:B:196:ASN:ND2	1:B:198:TYR:H	2.17	0.42
1:D:49:VAL:CG1	1:D:83:ALA:HB2	2.49	0.42
1:A:14:LEU:HD13	1:A:73:PRO:HG3	2.02	0.41
1:A:19:MET:HB3	1:A:19:MET:HE3	1.69	0.41
1:A:213:VAL:HG13	1:A:237:ALA:HB1	2.02	0.41
1:B:243:LYS:HG3	1:D:247:LEU:HG	2.02	0.41
1:C:134:PRO:O	1:C:137[B]:MET:HE2	2.18	0.41
1:C:137[A]:MET:HE2	2:C:284:H4M:N8	2.32	0.41
1:F:279:MET:HE3	1:F:279:MET:CA	2.48	0.41
1:F:198:TYR:HA	1:F:201:VAL:HG22	2.02	0.41
1:C:120:LYS:N	1:C:121:PRO:CD	2.83	0.41
1:A:137[A]:MET:HE3	1:A:137[A]:MET:HB3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:HE1	1:F:19:MET:CE	2.34	0.41
1:C:99:ASP:CG	1:C:101:PRO:HD2	2.46	0.41
1:C:128:ARG:HH21	2:C:284:H4M:H33	1.85	0.41
1:B:138:ALA:HB2	1:F:19:MET:HE2	2.02	0.41
1:C:39:GLY:HA3	6:C:335:HOH:O	2.21	0.41
1:D:227:LYS:O	1:D:231:VAL:HG23	2.21	0.41
1:F:19:MET:HB3	1:F:19:MET:HE3	1.73	0.41
1:A:97:ILE:HD12	1:A:117:ILE:HB	2.03	0.41
1:B:120:LYS:HB2	1:B:121:PRO:HD3	2.02	0.41
1:C:243:LYS:NZ	1:F:250:GLU:OE2	2.51	0.40
1:E:97:ILE:HD12	1:E:117:ILE:HB	2.03	0.40
1:B:19:MET:HE2	1:F:138:ALA:HB2	2.03	0.40
1:D:120:LYS:N	1:D:121:PRO:CD	2.85	0.40
2:A:284:H4M:H12	2:A:284:H4M:C13	2.51	0.40
1:B:38:VAL:HA	1:F:37:VAL:O	2.21	0.40
1:C:125:LEU:HD12	1:C:125:LEU:C	2.46	0.40
1:C:133:ASP:HB2	1:C:134:PRO:HD2	2.02	0.40
1:D:136:GLU:OE1	1:D:238:HIS:HD2	2.05	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:OE2	3:B:285:CA:CA[1_454]	1.29	0.91
1:B:89:ASP:OD2	1:E:50:GLU:OE2[1_656]	1.65	0.55
1:F:170:GLU:OE1	1:F:227:LYS:NZ[1_655]	1.94	0.26
1:B:177:ASP:OD2	1:E:170:GLU:OE1[1_556]	2.16	0.04
1:F:170:GLU:OE1	1:F:227:LYS:CE[1_655]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/283 (99%)	271 (96%)	10 (4%)	0	100	100
1	B	280/283 (99%)	270 (96%)	10 (4%)	0	100	100
1	C	283/283 (100%)	275 (97%)	8 (3%)	0	100	100
1	D	280/283 (99%)	273 (98%)	7 (2%)	0	100	100
1	E	280/283 (99%)	269 (96%)	11 (4%)	0	100	100
1	F	281/283 (99%)	271 (96%)	10 (4%)	0	100	100
All	All	1685/1698 (99%)	1629 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/234 (100%)	232 (99%)	2 (1%)	70	78
1	B	233/234 (100%)	229 (98%)	4 (2%)	53	62
1	C	236/234 (101%)	235 (100%)	1 (0%)	84	89
1	D	233/234 (100%)	230 (99%)	3 (1%)	61	69
1	E	233/234 (100%)	229 (98%)	4 (2%)	53	62
1	F	234/234 (100%)	232 (99%)	2 (1%)	70	78
All	All	1403/1404 (100%)	1387 (99%)	16 (1%)	65	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	280	GLU
1	B	2	THR
1	B	14	LEU
1	B	190	GLU
1	B	280	GLU
1	C	14	LEU

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Mol	Chain	Res	Type
1	D	2	THR
1	D	14	LEU
1	D	280	GLU
1	E	14	LEU
1	E	190	GLU
1	E	228	GLU
1	E	280	GLU
1	F	14	LEU
1	F	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	238	HIS
1	B	196	ASN
1	B	212	ASN
1	B	238	HIS
1	C	196	ASN
1	C	238	HIS
1	D	196	ASN
1	D	212	ASN
1	D	238	HIS
1	E	196	ASN
1	E	212	ASN
1	E	238	HIS
1	F	196	ASN
1	F	212	ASN
1	F	238	HIS
1	F	258	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	H4M	B	284	-	47,49,58	1.15	4 (8%)	58,74,86	2.44	22 (37%)
2	H4M	D	284	-	47,49,58	0.91	1 (2%)	58,74,86	2.53	17 (29%)
2	H4M	C	284	-	47,49,58	1.08	4 (8%)	58,74,86	1.75	10 (17%)
4	GOL	B	286	-	5,5,5	0.29	0	5,5,5	0.94	0
2	H4M	E	284	-	47,49,58	1.18	5 (10%)	58,74,86	1.77	13 (22%)
2	H4M	F	284	-	47,49,58	1.06	3 (6%)	58,74,86	2.22	11 (18%)
2	H4M	A	284	-	47,49,58	0.78	0	58,74,86	1.52	10 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H4M	B	284	-	-	11/27/71/85	0/5/5/5
2	H4M	D	284	-	-	5/27/71/85	0/5/5/5
2	H4M	C	284	-	-	6/27/71/85	0/5/5/5
4	GOL	B	286	-	-	2/4/4/4	-
2	H4M	E	284	-	-	6/27/71/85	0/5/5/5
2	H4M	F	284	-	-	5/27/71/85	0/5/5/5
2	H4M	A	284	-	-	9/27/71/85	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	284	H4M	C4A-C4	-3.34	1.35	1.43
2	E	284	H4M	C8A-N8	-3.00	1.32	1.35
2	C	284	H4M	CX1-CX2	3.00	1.56	1.53
2	B	284	H4M	C4A-N5	2.81	1.45	1.37
2	E	284	H4M	C4A-C4	-2.70	1.36	1.43
2	D	284	H4M	C4A-C4	-2.54	1.37	1.43
2	F	284	H4M	C7-N8	-2.43	1.44	1.47
2	C	284	H4M	C4A-C4	-2.39	1.37	1.43
2	C	284	H4M	C4-N3	-2.29	1.34	1.38
2	C	284	H4M	C6-N5	-2.27	1.44	1.47
2	B	284	H4M	OX5-C1J	2.24	1.43	1.40
2	F	284	H4M	OH4-C4	2.23	1.27	1.23
2	E	284	H4M	C10-N5	2.22	1.47	1.45
2	E	284	H4M	OX5-C1J	2.10	1.43	1.40
2	B	284	H4M	C10-N5	2.10	1.47	1.45
2	E	284	H4M	C8A-N1	-2.08	1.32	1.36
2	B	284	H4M	CX2-CX3	2.03	1.57	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	284	H4M	O4J-C1J-OX5	-12.25	98.51	111.95
2	F	284	H4M	O4J-C1J-OX5	-10.80	100.10	111.95
2	B	284	H4M	O4J-C1J-OX5	-8.89	102.19	111.95
2	D	284	H4M	C7-C6-N5	-5.83	102.79	108.61
2	B	284	H4M	C4A-C4-N3	5.62	120.84	110.94
2	C	284	H4M	C9M-C9-N10	-5.58	103.48	112.63
2	B	284	H4M	CX4-CX3-CX2	-5.28	104.78	113.57
2	F	284	H4M	C7-C6-N5	-5.24	103.39	108.61
2	E	284	H4M	O4J-C1J-OX5	-5.07	106.39	111.95
2	C	284	H4M	C7-C6-N5	-5.01	103.61	108.61
2	A	284	H4M	C7-C6-N5	-4.96	103.66	108.61
2	D	284	H4M	C4A-C4-N3	4.93	119.62	110.94
2	B	284	H4M	C7-C6-N5	-4.92	103.70	108.61
2	B	284	H4M	C7M-C7-N8	-4.77	104.87	109.44
2	F	284	H4M	OX5-C1J-C2J	4.76	115.41	107.81
2	C	284	H4M	C4A-C4-N3	4.63	119.09	110.94
2	A	284	H4M	C4A-C4-N3	4.56	118.96	110.94
2	D	284	H4M	C2-N1-C8A	4.51	121.32	113.36
2	D	284	H4M	OH4-C4-C4A	-4.48	116.64	127.62
2	E	284	H4M	CX4-CX3-CX2	-4.02	106.88	113.57
2	C	284	H4M	O4J-C1J-OX5	-3.97	107.59	111.95
2	B	284	H4M	C2-N1-C8A	3.95	120.33	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	284	H4M	OH4-C4-C4A	-3.93	117.96	127.62
2	B	284	H4M	OX3-CX3-CX4	-3.83	100.24	108.93
2	A	284	H4M	C2-N1-C8A	3.80	120.07	113.36
2	F	284	H4M	C4A-C4-N3	3.64	117.34	110.94
2	E	284	H4M	OX5-C1J-C2J	3.58	113.52	107.81
2	E	284	H4M	C4A-C4-N3	3.51	117.12	110.94
2	F	284	H4M	CX4-CX3-CX2	-3.41	107.89	113.57
2	D	284	H4M	C2-N3-C4	-3.41	118.93	125.11
2	A	284	H4M	O4J-C1J-OX5	-3.26	108.37	111.95
2	C	284	H4M	OH4-C4-C4A	-3.25	119.64	127.62
2	F	284	H4M	C2-N1-C8A	3.19	118.99	113.36
2	E	284	H4M	C7-C6-N5	-3.18	105.44	108.61
2	E	284	H4M	OX5-CX5-CX4	-3.17	102.02	109.29
2	B	284	H4M	O3A-PA-O2A	3.13	119.55	107.80
2	C	284	H4M	OX4-CX4-CX5	-3.13	103.08	109.99
2	C	284	H4M	C2-N1-C8A	3.08	118.79	113.36
2	E	284	H4M	C7M-C7-N8	-3.05	106.51	109.44
2	E	284	H4M	C9M-C9-N10	-3.05	107.63	112.63
2	B	284	H4M	C9M-C9-N10	-3.04	107.64	112.63
2	D	284	H4M	C7M-C7-N8	3.00	112.31	109.44
2	B	284	H4M	OH4-C4-C4A	-3.00	120.26	127.62
2	D	284	H4M	OX4-CX4-CX5	-2.87	103.66	109.99
2	A	284	H4M	C5J-C4J-C3J	-2.84	104.97	115.21
2	E	284	H4M	C2-N1-C8A	2.78	118.26	113.36
2	F	284	H4M	C7M-C7-N8	-2.76	106.80	109.44
2	B	284	H4M	C9-C6-N5	2.72	104.91	102.36
2	D	284	H4M	OX5-C1J-C2J	2.72	112.15	107.81
2	B	284	H4M	O3J-C3J-C2J	-2.72	103.11	111.82
2	E	284	H4M	OX2-CX2-CX3	-2.68	102.98	109.25
2	C	284	H4M	C2-N3-C4	-2.65	120.31	125.11
2	D	284	H4M	O2A-PA-O5J	-2.65	99.77	106.67
2	B	284	H4M	OX5-C1J-C2J	2.64	112.03	107.81
2	B	284	H4M	O3A-PA-O5J	-2.63	99.81	106.67
2	D	284	H4M	O3A-PA-O2A	2.61	117.60	107.80
2	D	284	H4M	OX4-CX4-CX3	-2.60	103.16	109.25
2	B	284	H4M	O3J-C3J-C4J	-2.50	103.90	111.08
2	A	284	H4M	OH4-C4-C4A	-2.47	121.56	127.62
2	D	284	H4M	CX5-CX4-CX3	2.47	116.87	112.22
2	F	284	H4M	OH4-C4-N3	2.43	124.68	120.11
2	B	284	H4M	O2A-PA-O5J	-2.38	100.47	106.67
2	E	284	H4M	O3J-C3J-C4J	-2.36	104.31	111.08
2	D	284	H4M	C5J-C4J-C3J	-2.34	106.77	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	284	H4M	C2-N3-C4	-2.32	120.90	125.11
2	A	284	H4M	C9M-C9-N10	-2.28	108.89	112.63
2	B	284	H4M	C2J-C3J-C4J	2.28	107.02	102.61
2	B	284	H4M	N3-C2-N1	-2.26	119.18	123.32
2	B	284	H4M	OX3-CX3-CX2	2.25	114.05	108.93
2	C	284	H4M	C10-N10-C14	2.25	127.55	120.41
2	E	284	H4M	O3A-PA-O2A	2.24	116.21	107.80
2	B	284	H4M	C15-C14-N10	-2.21	117.12	121.13
2	B	284	H4M	C2-N3-C4	-2.20	121.12	125.11
2	F	284	H4M	O3A-PA-O2A	2.16	115.90	107.80
2	D	284	H4M	O3J-C3J-C4J	-2.14	104.92	111.08
2	A	284	H4M	O5J-PA-O1A	-2.14	100.66	106.44
2	A	284	H4M	C7M-C7-N8	2.10	111.45	109.44
2	D	284	H4M	C9M-C9-N10	-2.06	109.26	112.63
2	E	284	H4M	OH4-C4-C4A	-2.05	122.59	127.62
2	D	284	H4M	C1J-C2J-C3J	2.04	104.83	102.29
2	B	284	H4M	C1J-O4J-C4J	2.04	113.53	105.76
2	A	284	H4M	C2-N3-C4	-2.03	121.42	125.11
2	C	284	H4M	C9-C6-N5	-2.01	100.47	102.36

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	284	H4M	O4J-C1J-OX5-CX5
2	A	284	H4M	C2J-C1J-OX5-CX5
2	A	284	H4M	C5J-O5J-PA-O2A
2	A	284	H4M	C5J-O5J-PA-O3A
2	B	284	H4M	O4J-C1J-OX5-CX5
2	B	284	H4M	C2J-C1J-OX5-CX5
2	B	284	H4M	C5J-O5J-PA-O2A
2	B	284	H4M	C5J-O5J-PA-O3A
2	C	284	H4M	O4J-C1J-OX5-CX5
2	C	284	H4M	C2J-C1J-OX5-CX5
2	C	284	H4M	C5J-O5J-PA-O1A
2	C	284	H4M	C5J-O5J-PA-O2A
2	D	284	H4M	O4J-C1J-OX5-CX5
2	D	284	H4M	C2J-C1J-OX5-CX5
2	E	284	H4M	O4J-C1J-OX5-CX5
2	E	284	H4M	C2J-C1J-OX5-CX5
2	E	284	H4M	C5J-O5J-PA-O1A
2	E	284	H4M	C5J-O5J-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	E	284	H4M	C5J-O5J-PA-O3A
2	F	284	H4M	O4J-C1J-OX5-CX5
2	F	284	H4M	C2J-C1J-OX5-CX5
2	F	284	H4M	C5J-O5J-PA-O2A
2	F	284	H4M	C5J-O5J-PA-O3A
4	B	286	GOL	O1-C1-C2-C3
2	A	284	H4M	OX3-CX3-CX4-OX4
4	B	286	GOL	O1-C1-C2-O2
2	A	284	H4M	OX3-CX3-CX4-CX5
2	B	284	H4M	OX3-CX3-CX4-CX5
2	B	284	H4M	OX3-CX3-CX4-OX4
2	A	284	H4M	CX2-CX3-CX4-CX5
2	B	284	H4M	CX2-CX3-CX4-CX5
2	A	284	H4M	CX2-CX3-CX4-OX4
2	B	284	H4M	CX2-CX3-CX4-OX4
2	A	284	H4M	C5J-O5J-PA-O1A
2	B	284	H4M	C5J-O5J-PA-O1A
2	F	284	H4M	C5J-O5J-PA-O1A
2	E	284	H4M	O4J-C4J-C5J-O5J
2	D	284	H4M	CX2-CX3-CX4-CX5
2	B	284	H4M	OX2-CX2-CX3-OX3
2	D	284	H4M	C5J-O5J-PA-O1A
2	C	284	H4M	C5J-O5J-PA-O3A
2	C	284	H4M	CX4-CX5-OX5-C1J
2	D	284	H4M	OX3-CX3-CX4-CX5
2	B	284	H4M	C3J-C4J-C5J-O5J

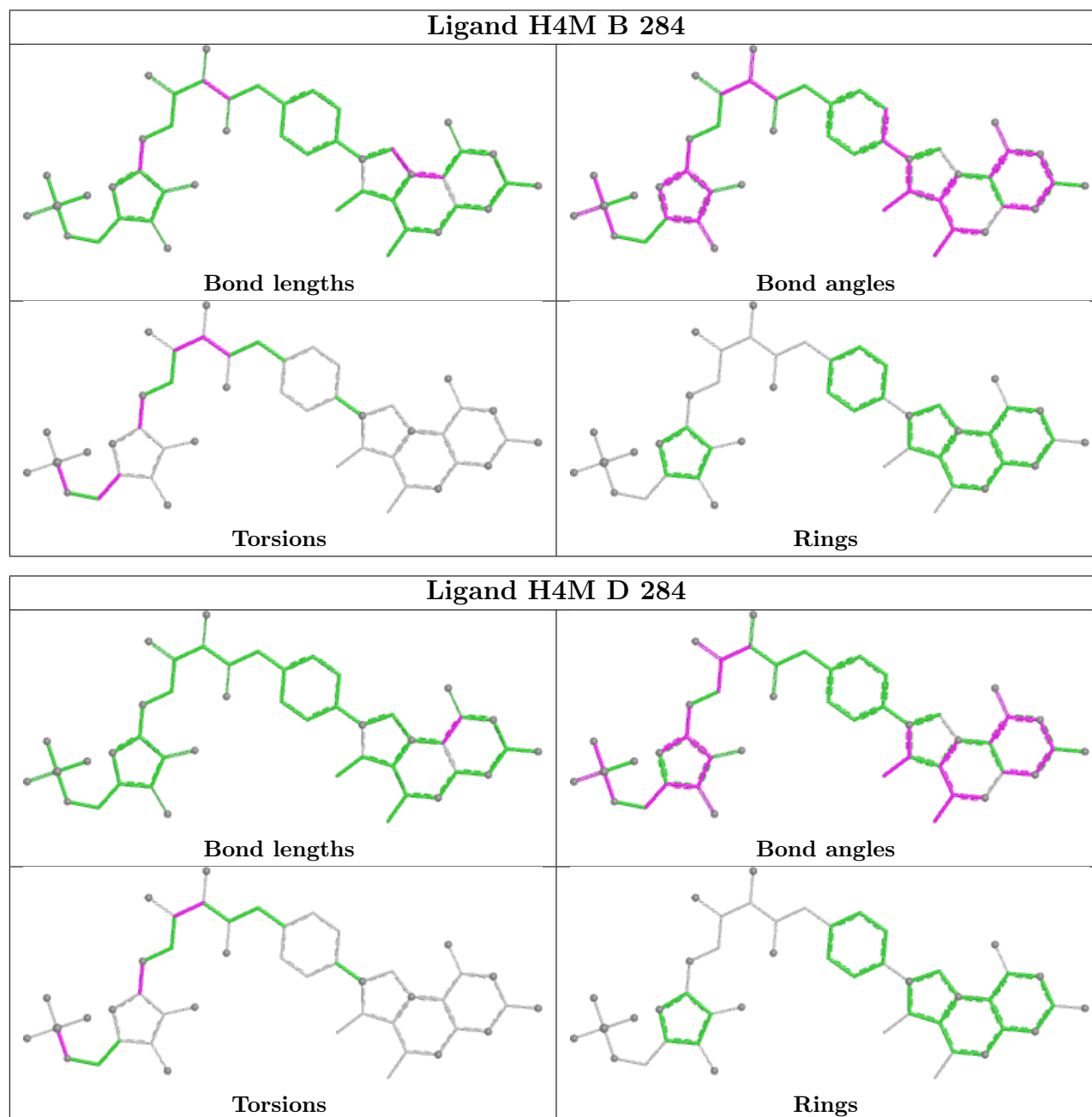
There are no ring outliers.

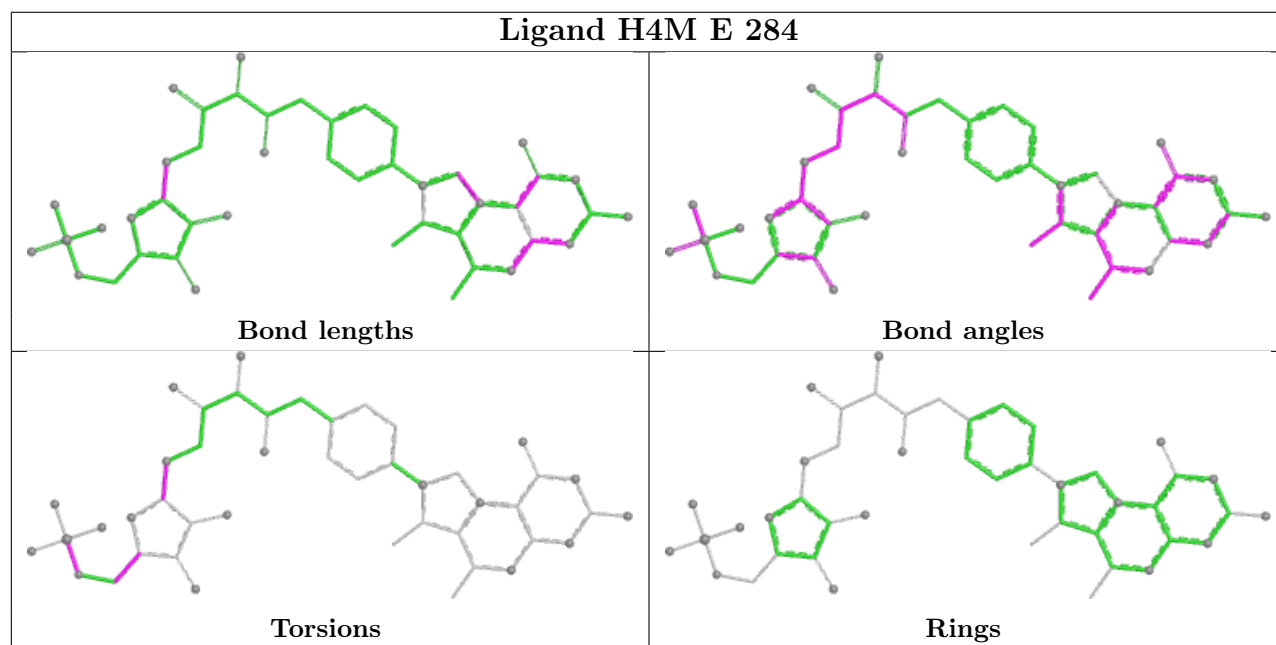
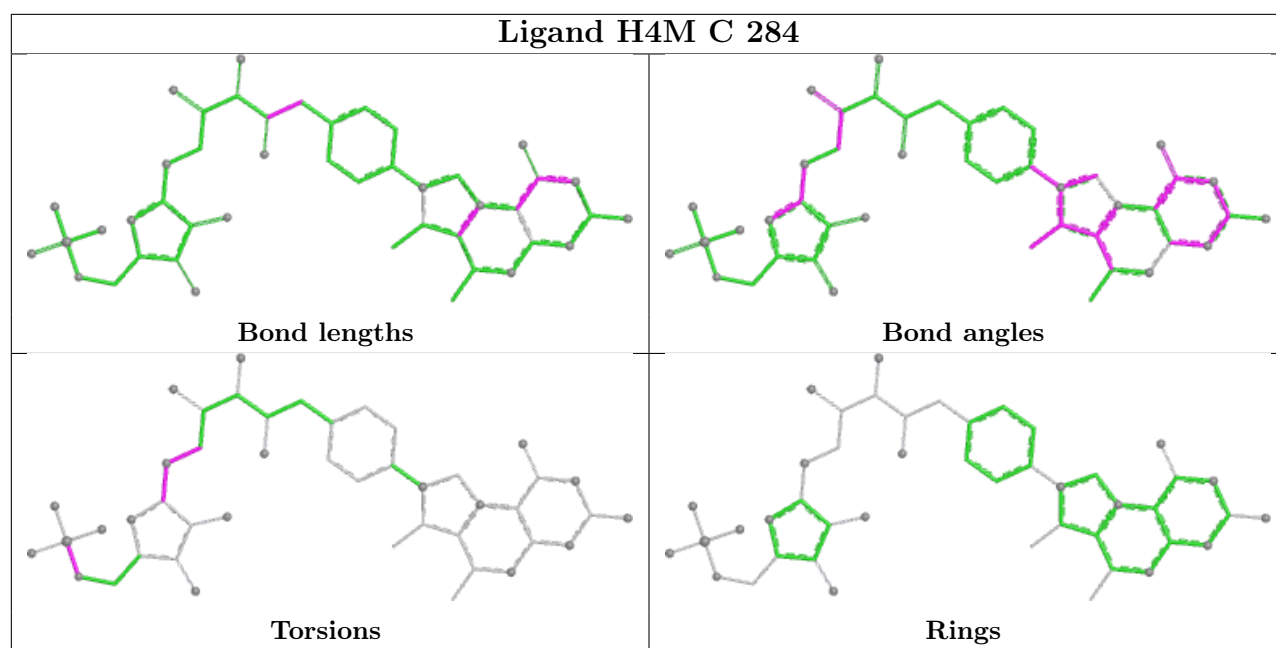
6 monomers are involved in 37 short contacts:

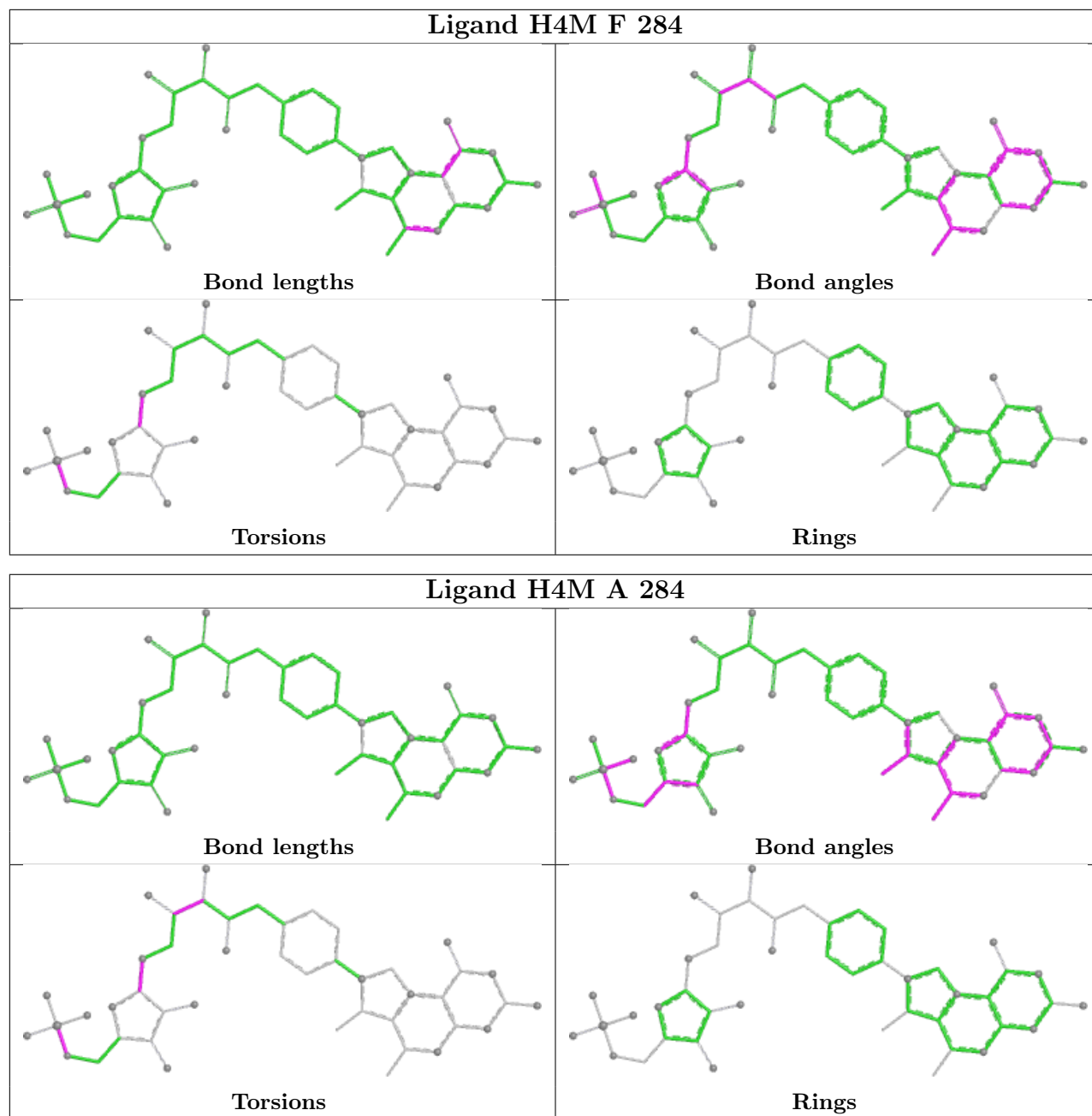
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	284	H4M	6	0
2	C	284	H4M	12	0
4	B	286	GOL	3	0
2	E	284	H4M	1	0
2	F	284	H4M	7	0
2	A	284	H4M	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	282/283 (99%)	0.93	48 (17%) 4 4	2, 8, 21, 43	1 (0%)
1	B	282/283 (99%)	0.34	9 (3%) 50 53	2, 8, 21, 43	1 (0%)
1	C	282/283 (99%)	0.44	12 (4%) 40 41	2, 8, 21, 43	4 (1%)
1	D	282/283 (99%)	0.94	36 (12%) 7 8	2, 8, 21, 43	0
1	E	282/283 (99%)	0.12	3 (1%) 78 80	2, 8, 21, 43	0
1	F	282/283 (99%)	0.15	4 (1%) 73 75	2, 8, 21, 43	2 (0%)
All	All	1692/1698 (99%)	0.49	112 (6%) 24 26	2, 8, 22, 43	8 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	LEU	4.9
1	A	197	PRO	4.7
1	B	171	ASP	4.5
1	A	198	TYR	4.2
1	A	260	ALA	4.2
1	A	171	ASP	4.1
1	D	223	VAL	4.0
1	D	237	ALA	3.8
1	D	226	ASP	3.8
1	E	171	ASP	3.8
1	D	233	ILE	3.4
1	C	47	GLU	3.4
1	A	261	VAL	3.4
1	A	256	LYS	3.4
1	A	199	ALA	3.3
1	C	171	ASP	3.3
1	A	257	SER	3.2
1	D	257	SER	3.1
1	A	3	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	3.1
1	C	201	VAL	3.1
1	A	253	GLU	3.1
1	A	77	ALA	3.0
1	A	278	PHE	3.0
1	C	173	ILE	3.0
1	A	170	GLU	3.0
1	C	91	GLU	3.0
1	D	173	ILE	3.0
1	D	63	PHE	3.0
1	D	171	ASP	2.9
1	D	236	SER	2.9
1	B	62	ASP	2.9
1	B	91	GLU	2.9
1	A	194	PHE	2.9
1	A	76	ALA	2.9
1	D	210	ALA	2.8
1	F	170	GLU	2.7
1	C	63	PHE	2.7
1	D	232	PRO	2.7
1	D	279	MET	2.7
1	A	58	ASP	2.7
1	A	12	GLY	2.7
1	A	271	LYS	2.7
1	A	46	PRO	2.7
1	D	282	PRO	2.7
1	B	170	GLU	2.7
1	A	113	GLY	2.7
1	A	111	GLU	2.6
1	F	89	ASP	2.6
1	D	170	GLU	2.6
1	E	170	GLU	2.6
1	D	222	PHE	2.5
1	D	218	VAL	2.5
1	D	231	VAL	2.5
1	C	54	GLU	2.5
1	D	205	ALA	2.5
1	D	71	GLY	2.5
1	D	229	ARG	2.5
1	A	259	ASP	2.5
1	A	47	GLU	2.5
1	E	172	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	ALA	2.5
1	D	266	HIS	2.5
1	A	258	ASN	2.5
1	C	50	GLU	2.4
1	A	248	ALA	2.4
1	B	2	THR	2.4
1	A	57	LEU	2.4
1	A	262	LEU	2.4
1	D	235	ALA	2.3
1	A	201	VAL	2.3
1	A	196	ASN	2.3
1	A	114	LEU	2.3
1	B	54	GLU	2.3
1	B	172	GLU	2.3
1	D	228	GLU	2.3
1	A	282	PRO	2.3
1	C	282	PRO	2.3
1	B	245	ALA	2.3
1	C	45	ASP	2.3
1	D	227	LYS	2.3
1	D	240	MET	2.3
1	A	173	ILE	2.2
1	D	123	ALA	2.2
1	D	200	MET	2.2
1	C	254	LEU	2.2
1	D	247	LEU	2.2
1	D	111	GLU	2.2
1	D	199	ALA	2.2
1	A	264	THR	2.2
1	A	89	ASP	2.2
1	D	45	ASP	2.2
1	A	85	GLU	2.2
1	D	269	ASP	2.2
1	D	201	VAL	2.1
1	A	115	GLY	2.1
1	A	273	LEU	2.1
1	A	92	TYR	2.1
1	C	170	GLU	2.1
1	A	82	LYS	2.1
1	A	56	ALA	2.1
1	D	262	LEU	2.1
1	F	173	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	SER	2.1
1	A	244	ALA	2.1
1	B	60	ALA	2.1
1	F	2	THR	2.0
1	A	231	VAL	2.0
1	A	206	ALA	2.0
1	A	267	ALA	2.0
1	D	57	LEU	2.0
1	D	254	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

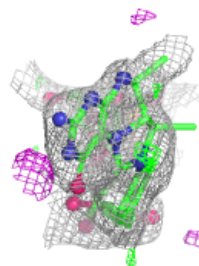
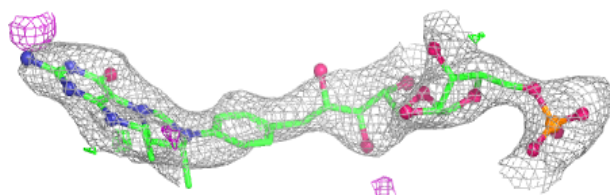
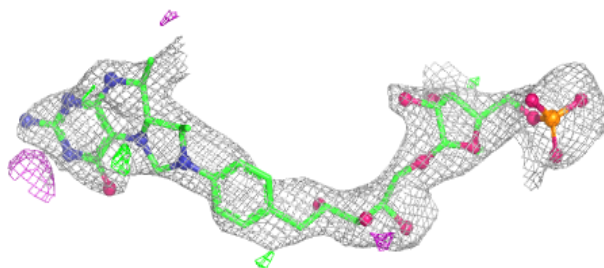
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	D	285	1/1	0.71	0.15	45,45,45,45	0
5	NA	E	285	1/1	0.73	0.33	72,72,72,72	0
4	GOL	B	286	6/6	0.80	0.16	53,57,58,62	0
5	NA	F	285	1/1	0.81	0.26	58,58,58,58	0
2	H4M	A	284	45/54	0.83	0.18	56,63,75,77	45
2	H4M	B	284	45/54	0.85	0.13	32,39,70,74	0
2	H4M	D	284	45/54	0.87	0.14	32,43,64,67	45
2	H4M	C	284	45/54	0.89	0.12	28,38,63,65	45
2	H4M	E	284	45/54	0.91	0.10	34,41,66,72	0
2	H4M	F	284	45/54	0.93	0.09	26,40,77,79	0
3	CA	B	285	1/1	0.97	0.05	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

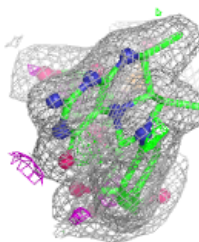
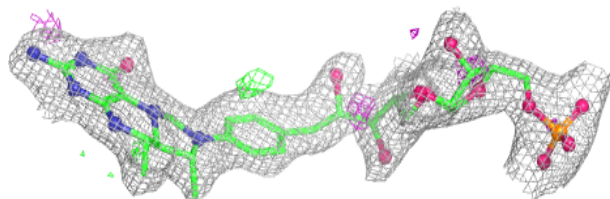
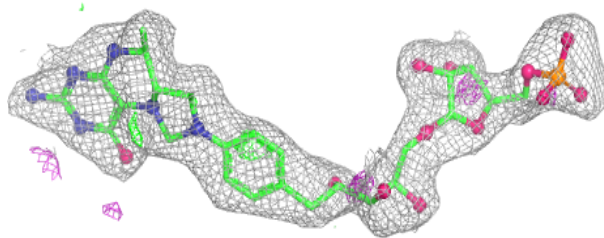
Electron density around H4M A 284:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



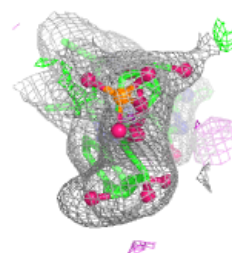
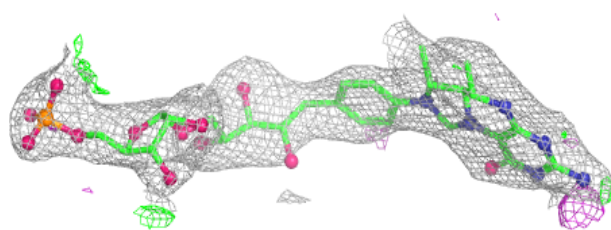
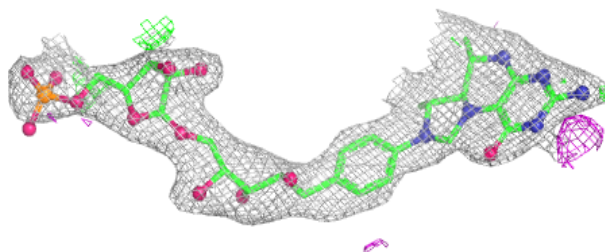
Electron density around H4M B 284:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

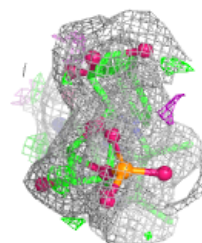
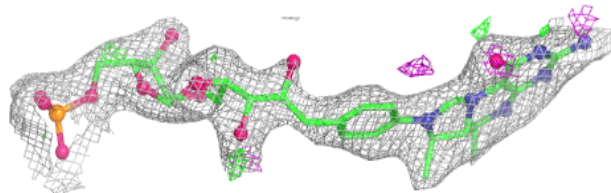
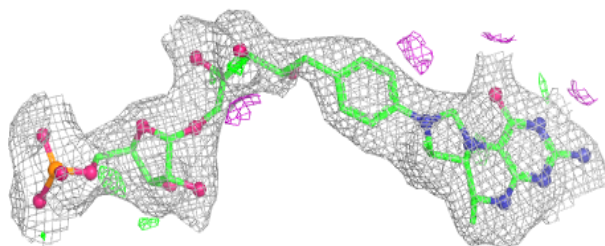


Electron density around H4M D 284:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

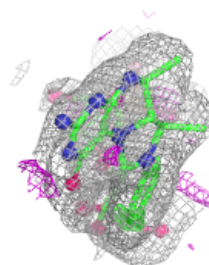
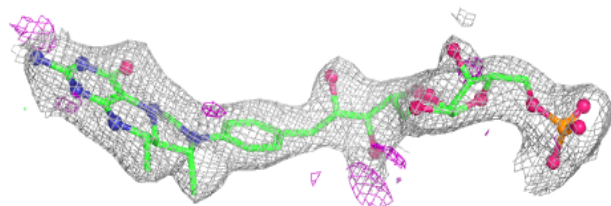
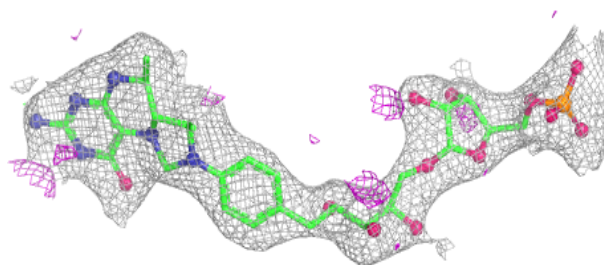
**Electron density around H4M C 284:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

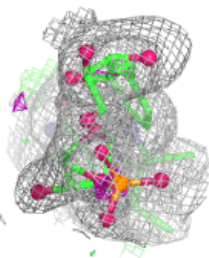
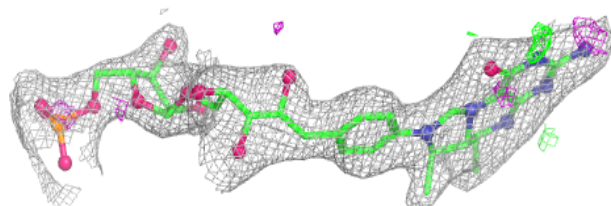
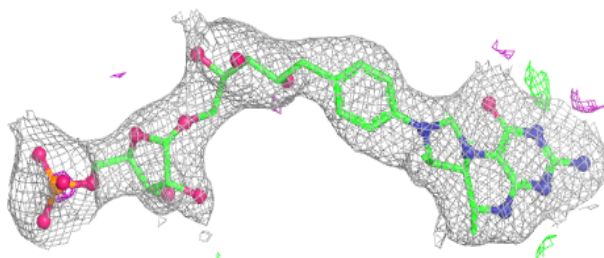


Electron density around H4M E 284:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around H4M F 284:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.